Ayush Asthana

Current Position:	Postdoctoral Research Associate in Quantum Computing
Department, University:	Department of Chemistry, Virginia Tech
Contact:	ayushasthana15@gmail.com, +1 443-708-6400
LinkedIn Profile:	linkedin.com/in/ayushasthana
GitHub Profile:	github.com/aasthan4, github.com/asthanaa
Personal website:	aasthan4.github.io/
Research Interest:	Quantum Chemistry, Quantum Information Science, Quantum Control

Employment

Aug 2021-current — **Postdoctoral Research Associate, Virginia Tech**
Advisor: Prof. Nicholas J. Mayhall
- Quantum computing using principles of quantum control theory
- Quantum chemistry on near-term quantum computers

May 2014-Jul 2014 — **Undergraduate Summer Research Intern**
Advisor: Prof. T. Daniel Crawford
- Computational study of optical rotation in molecules and theoretical chemistry summer school

Education

Aug 2016-Jul 2021 — **PhD in Theoretical Chemistry, Johns Hopkins University**
Advisor: Prof. Lan Cheng
Dissertation: Development of relativistic quantum chemistry methods for heavy-element containing molecules

Jul 2011- May 2016 — **BS-MS Dual Degree in Chemistry, Indian Institute of Technology Kanpur**
Advisors: Prof. Debashis Mukherjee (IACS), co-advisor: Prof. Srihari Keshavamurthy (IITK)
Thesis: Treatment of Bond Breaking and handling of Quasi-Degeneracy: Formulation of a multi-reference analog of Single reference Perturbation Theory of 2nd order

Certifications

Jul 2020 — Global Summer School on Quantum Computing by IBM (Certificate)

May 2020 — Professional certificate in Quantum Computing and Quantum Internet
Delft University of Technology in collaboration with edX

Pre-publications (Submitted for Peer-review)

*- corresponding author

1. A. Kumar*, **A. Asthana**, V. Abraham, T. Crawford, N. Mayhall, Y. Zhang, L. Cincio, S. Tretiak, P. Dub*, "Quantum simulation of molecular response properties", arxiv.org/abs/2301.06260 (Under review at Chemical Science, RSC) (2022).
2. **A. Asthana**, C. Liu, O. R. Meitei, S. E. Economou, E. Barnes, N. J. Mayhall*, "Minimizing state preparation times in pulse-level variational molecular simulations", arxiv.org/abs/2203.06818 (just accepted at Physical Review Applied) (2023).

Publications (Peer-reviewed)

3. **A. Asthana*** A. Kumar, V. Abraham, H. Grimsley, Y. Zhang, L. Cincio, S. Tretiak, P. Dub, S. Economou, E. Barnes, N. Mayhall*, "quantum self-consistent equation-of-motion method for computing molecular excitation energies, ionization potentials, and electron affinities", Chem. Sci., **14**, 2405 (2023).
4. A. Kumar*, **A. Asthana**, C. Masteran, E. F. Valeev, Y. Zhang, L. Cincio, S. Tretiak, P. A. Dub*, "Accurate quantum simulation of molecular ground and excited states with a transcorrelated Hamiltonian", J. Chem. Theory Comput. **18**, 9, 5312 (2022).
5. J. Liu, X. Zheng, **A. Asthana**, C. Zhang, and L. Cheng*, "Analytic Evaluation of Energy First Derivatives for Spin-Orbit Coupled-Cluster Singles and Doubles Augmented with Noniterative Triples Method: General Formulation and An Implementation for First-Order Properties", J. Chem. Phys. **154**, 064110 (2021).
6. G. Liu, C. Zhang, S. Ciborowski, **A. Asthana**, L. Cheng* and K. Bowen*, "Mapping the Electronic Structure of the Uranium (VI) Dinitride Molecule, UN2", J. Phys. Chem. A, **124**, 6486 (2020).
7. **A. Asthana**, J. Liu, and L. Cheng*, "Exact two-component equation-of-motion coupled-cluster singles and doubles method using atomic mean-field spin-orbit integrals", J. Chem. Phys. **150**, 074102 (2019).
8. J. Liu*, **A. Asthana***, L. Cheng*, and D. Mukherjee*, "Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications",J. Chem. Phys. **148**, 244110 (2018).

9. J. Liu, Y. Shen, **A. Asthana**, and L. Cheng*, "Two-component relativistic coupled-cluster methods using mean-field spin-orbit integrals", J. Chem. Phys. **148**, 034106 (2018).

Presentations

Invited

1. Quantum Brilliance, Germany, Feb 2023, "Towards molecular simulation on near-term quantum computers".
2. VTQ symposium, Virginia Tech, Feb 2023 "Pulse-level molecular simulation algorithms for near-term quantum computers".
3. VTQ internal seminar, Virginia Tech, Dec 2022, "Path to quantum chemistry on near-term quantum computers".
4. Applied Physics Lab, Johns Hopkins University, Nov 2022, "Pulse-level molecular simulation on transmon qubits".
5. Quantinuum (Honeywell), UK, Oct 2022, "Towards quantum chemistry on near-term quantum computers".
6. Oak Ridge National Lab, Jul 2022, "Pulse-level variational molecular simulation".
7. Virginia Tech, Mar 2021, "Relativistic coupled-cluster methods for heavy-element-containing molecules".
8. IBM Almaden Research Center, Jul 2020, "Relativistic quantum chemistry methods for heavy-element computational chemistry".

Contributed

9. American Physical Society National Meeting Las Vegas, NV Mar 2023, "Role of orbital-optimization molecular ground and excited-state calculations on quantum computer (Oral presentation)".
10. American Chemical Society National Meeting Chicago, IL Aug 2022, "Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Oral presentation)".
11. American Chemical Society National Meeting Chicago, IL Aug 2022, "Minimizing pulse level variational molecular simulation (Oral presentation)".
12. Molecular Quantum Mechanics (MQM), Blacksburg, Jun 2022, "Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Poster presentation)".
13. Quantum Information Science symposium at Virginia Tech, Apr 2022, "Pulse-level variational molecular simulation (Oral presentation)".
14. American Physical Society National Meeting Chicago, IL Mar 2022, "Minimizing state preparation times in pulse-level variational molecular simulation (Oral presentation)".
15. American Chemical Society National Meeting & Exposition, San Francisco, CA, Aug 2020, "New algorithmic development for relativistic equation-of-motion coupled-cluster method (Poster presentation)".
16. Johns Hopkins University, Dec 2019, "Development of relativistic quantum chemistry methods for molecules containing heavy-elements (Graduate Board Oral talk)".
17. Johns Hopkins University, Mar 2019, "Chemistry at ultracold temperatures (Department seminar)".
18. Indian Institute of Technology Kanpur, Apr 2016, "Extended wick's theorem, spin-free cumulants and their role in the formulation and analyzing spacial and spin correlation of many-electron systems (Master's thesis talk)".

by collaborators

19. Zhao T. et. al., Gate-free VQE Exploiting Inter-qubit Parametric Interaction (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023
20. Kumar A. et. al., Accurate quantum chemistry calculations using NISQ era quantum computers (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023
21. Liu C. et. al., Implementing pulse-based VQE (ctrl-VQE) algorithm on NISQ devices. (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023

Media

- Quantum researchers collide, Virginia Tech, Exponentially More

Achievements and Services

2020 to currently	Reviewer in NPJ Quantum Information (Nature), Chemical Science (RSC), Journal of chemical theory and computation (ACS), ACS Central Science.
Jan-May 2023	Co-organized Virginia Tech Quantum (VTQ) seminar series
Dec 2022	Committee member for masters thesis defence of a visiting student at Virginia Tech in Crawford lab.
April 2022	Co-organized Virginia Tech Quantum (VTQ) symposium, a two day symposium with more than 40 participants from the department of Physics, Computer Science and Chemistry
May 2016	Recepient of best master's project award, Department of Chemistry, IIT Kanpur.
2011-2016	Awarded *INSPIRE-SHE Scholarship* worth $6000, Department of Science and Technology, Government of India.
May 2011	Secured a position in the top 1% All India Rank in IIT-JEE 2011 competitive exam with more than 500,000 participants.
May 2011	Secured a top 0.2% All India Rank in AIEEE 2011 and UPTU 2011 competitive exams with over 1.1 million and 0.5 million participants, respectively.

Software Contributions

CFOUR	- Contributor in CFOUR (Coupled-Cluster techniques for Computational Chemistry) chemistry program, an international collaborative program for high accuracy molecular calculations. - Contributed an efficient implementation of relativistic spin-orbit coupled-cluster methods for calculations of molecules containing heavy elements.
AutoGen	- Developed open-sourced python-based automatic expression generator package for quantum chemical theories. - The program used wick's theorem to automatically derive working expressions. Deriving hundreds of these expressions, as in the case of unitary coupled-cluster (UCC) theory, can be time-taking and error-prone when done by hand.
Adapt-vqe	- Contributed methods for molecular excited-state energy (QSE, qEOM and q-sc-EOM) using simulations of adapt-VQE algorithm for ground-state wavefunction. - Resulted in two scientific publications.